Indian J. Phys. **81** (1) 125-129 (2007)

IJP

Electrical resistivity of liquid K-Rb-Cs alloys

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Abstracts : A model potential consisting of varying cancellation of attractive and repulsive potentials within the core is applied for the first time to study the electrical resistivity of liquid K-Rb-Cs alloys The influence of exchange and correlation effects are also studied by including local-field correlation functions due to Hartree, Taylor, Ichimaru-Utsumi, Farid *et al* and Sarkar *et al* The results for electrical resistivity of pure metallic components (K, Rb and Cs), liquid binaries (K-Rb, Rb-Cs and K-Cs) and liquid ternary (K-Rb-Cs) favours the formulation of our new model potential The comparison of present results with those obtained due to self-consistent energy independent model potential and experimental findings also confirm the validity of our model in the study of ternary alloys

Keywords : Pseudopotential, electrical resistivity, alloys

PACS Nos. : 71 15H, 72 15 Cz

1. Introduction

Alloys, the investigation of which is a general topic now days, are materials of common interest for scientist and researchers. Recently, ternary and quaternary alloy combinations have been of prime importance. The electrical resistivity and absolute thermoelectric power of liquid Indium-Nickel-Manganese ternary alloy was calculated by Auchet *et al.* [1], following the Fiber-Ziman formalism [2]. For simple liquid metals, structural and electrical properties were also studied significantly over the past few decades [3–6]. Khajil [7] has calculated the electrical resistivity of alkali-based binary alloys using the Faber-Ziman method modified for mean free-path. However the investigation related to multi component liquid metallic alloys of simple metals is still to be explored fully under the Fiber-Ziman formulation and pseudopotential theory. It was also pointed out by Jin *et al.* [8] that the Ziman type theory can be applied successfully in the prediction of the electronic transport properties for simple binary alloy systems but a close examination of its applicability to multicomponent systems is still needed. These all motivated us to consider further application of the pseudopotential theory to study

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electrical resistivity of alloys containing three different simple metallic constituents K-Rb-Cs, using our model potential [9,10]. The model pseudopotential has been successfully applied previously to the calculation of electronic properties of alkali metals and their binary alloys [10]. The influence of exchange and correlation effects are also investigated by including local field correlation functions due to Hartree (H) [11], Taylor (T) [12], Ichimaru-Utsumi (IU) [13], Farid *et al.* (F) [14] and Sarkar *et al.* (S) [15].

2. Interatomic pair potentials

The effective interatomic interaction for the ternary alloy system A-B-C can be written as [9,10],

$$V(r)=\left(\frac{Z^2e^2}{r}\right)+\frac{\Omega_o}{\pi^2}\int F(q)\left[\frac{\mathrm{Sin}(qr)}{qr}\right]q^2\,dq\,, \tag{1}$$

where $F(q)$ is the energy wave number characteristics. Also Z and Ω_0 are the effective valence and atomic volume of the ternary alloy system, respectively. It is noted by Jin *et al* [8] and Alblas *et al* [16] that such calculated Ω_0 do not contain serious error as indicated by the fact that the maximum volume contractions are 1.0% for K-Cs and 5.7% for Na-Cs.

3. Electrical resistivity

The expressions for the electrical resistivity for liquid metals, binary and ternary alloys are given by [8]

$$\rho=\left(\frac{3\pi\Omega}{4k_F^6}\right)\int_0^{2k_F}dqq^3\left[\sum_{i=1}^{3}C_ia_{ii}(q)|W_i(q)|^2+2(C_1C_2)^{1/2}a_{12}(q)W_1(q)W_2(q)\right.$$
$$\left.+2(C_1C_3)^{1/2}a_{13}(q)W_1(q)W_3(q)+2(C_2C_3)^{1/2}a_{23}(q)W_2(q)W_3(q)\right]. \tag{2}$$

Here, $a_{ij}(q)$ is the partial-structure factors and $W_i(q)$ the screened form factors, calculated with exchange-correlation effects included for the i-type ion in the alloy with different concentration.

Figure 1 shows the electrical resistivity of binary combinations K-Rb, K-Cs and Rb-Cs investigated for full range of concentration.

The computed electrical resistivity for the ternary K-Rb-Cs liquid alloys at 100°C are summarized in Table 1, along with the theoretical results obtained by Jin *et al* [8] using self-consistent energy independent model potential (SC-EIMP).

For liquid K and Cs, the computed resistivity due to F [14] local field correlation functions generates good agreement with the experimental findings [17–19]. While for Rb, the results due to S [15] screening function gives excellent agreement with experimental data [17–19].

The comparison with the results of SC-EIMP calculation of Jin *et al* [8] also

Table 1. The electrical resistivities calculated for K-Rb-Cs alloys at various concentrations C_i at 100°C. The bracketed values show the percentage deviation with respect to the Experimental value.

Alloys	C_K	C_{Rb}	C_{Cs}	r_c (a.u.)	Ω_0 (a.u.)	Present calculations with different local field correlation function					Expt. [17–19]	SC-EIMP Jin *et al* [8]
						ρ_H (μΩ cm)	ρ_T (μΩ cm)	ρ_{IU} (μΩ cm)	ρ_F (μΩ cm)	ρ_S (μΩ cm)		
K-Rb-Cs	0.6	0.2	0.2	2.8580	551.52	16.73	39.42	44.45	55.75	37.89		31.80
	0.4	0.2	0.4	3.0488	604.34	21.40	47.99	53.05	57.89	36.66		40.48
	0.4	0.4	0.2	2.8883	568.82	18.68	41.09	45.95	54.62	36.75		33.23
	0.2	0.2	0.6	3.3296	657.16	24.68	58.21	63.20	73.01	46.06		45.84
	0.2	0.4	0.4	3.0791	621.64	19.92	45.79	50.71	55.78	34.73		40.55
	0.2	0.6	0.2	2.9185	586.12	19.63	42.59	47.61	51.91	33.92		34.14

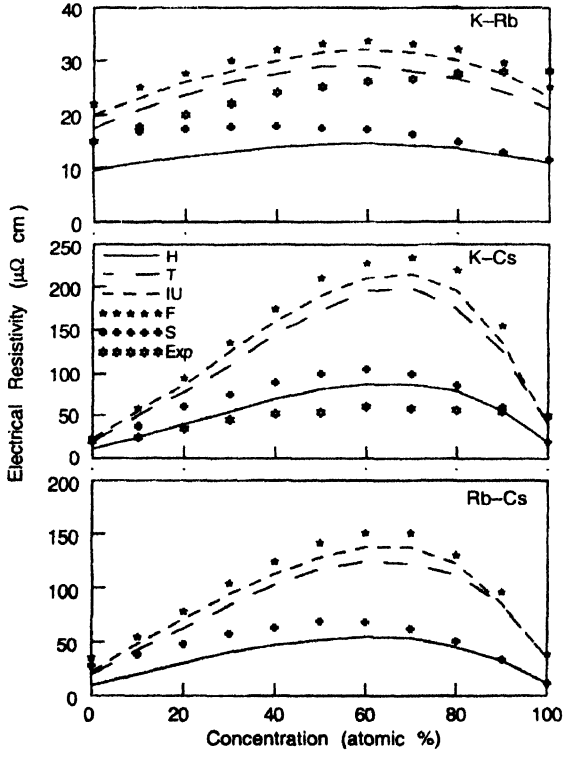

Figure 1. The computed electrical resistivity of K-Rb, K-Cs and Rb-Cs binary alloys along with Experimental data.

favours our results. For liquid K, Rb and Cs, the deviation of present findings from experimental data [17–19] is 0.5% to 16%, while for SC-EIMP [8] findings, such deviation is 9% to 84%.

For liquid binaries K-Rb, K-Cs and Rb-Cs, the highest resistivity is obtained for $K_{0.7}Cs_{0.3}$, which is also supported by experimental data [17–19]. In the SC-EIMP

calculation of Jin *et al* [8] resistivity of binaries increases with increase in atomic volume of the alloy and highest resistivity was obtained for $K_{0.2}Cs_{0.8}$ which is in contrast to experimental observation [17–19].

There is a pronounced maximum in the binary K-Cs alloys located at the highest atomic concentrations of the heavier elements *i.e.* at about 60–70 atomic % of Cs. Such a maximum also appears for liquid K-Rb-Cs system, when the concentration of Rb is set to 20 atomic %. The resistivity of K-Rb-Cs ternary increases substantially from K-rich alloy to Rb-rich alloys and to Cs-rich alloys. It is also predictable that, the presently computed electrical resistivity of ternary K-Rb-Cs systems changes smoothly with the concentration of each component and form a well defined "electrical resistivity surface" at 100°C as shown in Figure 2.

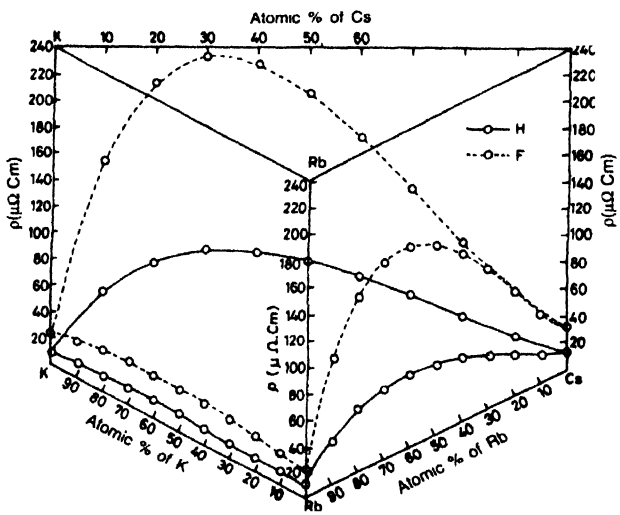

Figure 2. The electrical resistivity surface of ternary K-Rb-Cs alloys at 100°C.

It is found that comparing to static screening of Hartree [11], the local field correlation function due to F [14] affects the results of electrical resistivity very largely. The influence of various local field correlation functions on the resistivity with respect to static H [11] dielectric function for K-Rb alloys are 95–102% for T [12], 119–126% for IU [13], 133–142% for F [14] and 63–1% for S [15] screening functions. Such screening influence for K-Cs alloys are 139–102% for T [12], 143–126% for IU [13], 173–142% for F [14] and 47–1% for S [15] screening. Similarly, for Rb-Cs alloys, the screening influences are 139-95% for T [12], 143-119% for IU [13], 173–133% for F [14] and 1–63% for S [15], respectively.

We have also computed the effect of screening on the ternary K-Rb-Cs alloys. The deviation with respect to H [11] are 116-135% for T [12], 142-165% for IU [13], 164-233% for F [14] and 71–126% for S [15] screening functions.

We observed that, among the presently calculated resistivities, the ρ calculated by H [11] function is giving lower value while that of F [14] gives higher value. Hence

in the resistivity surface, the results due to these two screening functions are plotted.

4. Conclusions

The present model potential is proved capable of explaining the electrical resistivities of pure metals, binary alloys and ternary alloys The computed resistivities for the ternary alloys form an "electrical resistivity surface" in the full range of concentration. It is also concluded that, the Ziman type formulation along with the pseudopotential theory are found applicable in the study of electrical resistivities of the multi-component alloys

Acknowledgment

The work is supported under DRS/SAP of UGC, New Delhi SRM also acknowledges the support of UGC for providing DRS/SAP Fellowship

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